Nuclear Structure and Response based on Correlated Realistic Interactions

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Overview

- Introductory remarks
- The UCOM correlated Hamiltonian: a “tamed” realistic interaction
- UCOM-Hartree-Fock + long-range correlations

  Hartree-Fock and perturbation theory

  Hartree-Fock and RPA

  Extended RPA - the RPA ground state and excitations built on it
- Perspectives

The Nuclear Many-Body Problem

- Nuclear structure and dynamics starting from the NN interaction
  - Nuclei and Nuclear Matter (NM) described as systems of interacting Fermions - non-relativistic approach
- Fully microscopic calculations: only possible for light nuclei and NM, using advanced Quantum Many-Body Theory
  - GFMC: $A \leq 12$
- For heavier nuclei, we depend upon shell model, mean-field approaches

*** Effective NN interaction

NN interaction and simple Hilbert spaces

- Phenomenological effective interaction
  - limited predictive power (in our expanding nuclear landscape!)
- Derived from the bare NN interaction *(realistic potentials)*
  - [Brückner G-Matrix]
  - RG - low-momentum expansion: $V_{\mathrm{low}-k}$ potential employed in shell-model calculations
  - the UCOM Hamiltonian
  - ✌ *Possibility to combine realistic interactions with simple Hilbert spaces*

The Unitary Correlation Operator Method (UCOM)

- “A unitary correlation operator method”; H. Feldmeier, T. Neff, R. Roth and J. Schnack, Nucl. Phys. A 632 (1998) 61.
- “Tensor correlations in the unitary correlation operator method”; T. Neff and H. Feldmeier, Nucl. Phys. A 713 (2003) 311.
- “Nuclear Structure based on Correlated Realistic NN-Potentials”, R. Roth, T. Neff, H. Hergert and H. Feldmeier, Nucl. Phys. A 745 (2004) 3.
- More publications, presentations, theses, available on: http://crunch.ikp.physik.tu-darmstadt.de/tnp/ and http://www.gsi.de/forschung/tp/ .

The limitations of a Slater-Determinant Wavefunction: the Independent - Particle Model (IPM) breaks down in small-medium NN distances

- Short-range central correlations: pair distribution vanishes in small relative distance due to strong repulsive core

- Tensor correlations: distribution of particles depends also on relative spin orientation

The limitations of a Slater-Determinant Wavefunction: the Independent - Particle Model (IPM) breaks down in small-medium NN distances

introduce correlations by means of Unitary Correlation Operator (UCO) C acting on relative coordinates of all pairs:

$$C = \exp[-\mathrm{i}G] = \exp[-\mathrm{i}\sum_{i<j} g_{ij}] \ ; \ g_{ij} = g(\vec{r}_{ij}, \vec{q}_{ij}, \vec{\sigma}_i, \vec{\sigma}_j, \vec{\tau}_i, \vec{\tau}_j)$$

- Short-range central correlations: pair distribution vanishes in small relative distance due to strong repulsive core

  radial shift in the relative coordinate of nucleon pair:

$$C_r \ \leftrightarrow \ g_r = \tfrac{1}{2}[s(r)q_r + q_r s(r)] \ ; \ q_r = \tfrac{1}{2}[\tfrac{\vec{r}}{r}\vec{q} + \vec{q}\tfrac{\vec{r}}{r}]$$

- Tensor correlations: distribution of particles depends also on relative spin orientation

  angular shift depending on orientation of spin and relative coordinate:

$$C_\Omega \ \leftrightarrow \ g_\Omega = \tfrac{3}{2}\vartheta(r)[(\vec{\sigma}_i \cdot \vec{q}_\Omega)(\vec{\sigma}_j \cdot \vec{r}) + (\vec{r} \leftrightarrow \vec{q}_\Omega)] \ ; \ \vec{q}_\Omega = \vec{q} - \tfrac{\vec{r}}{r} q_r$$

UCO: $C = C_\Omega C_r = \exp[-\mathrm{i}G] \ ; \ G^\dagger = G \ ; \ C^\dagger C = 1$

Important aspects

- Unitary Operators

  Correlated wavefunctions or correlated operators

- Applied to a realistic NN hamiltonian:

  An effective interaction, which is:

  - "tamed" at short distances
  - given in explicit operator form - analytical calculations possible
  - phase-shift equivalent to the original bare interaction

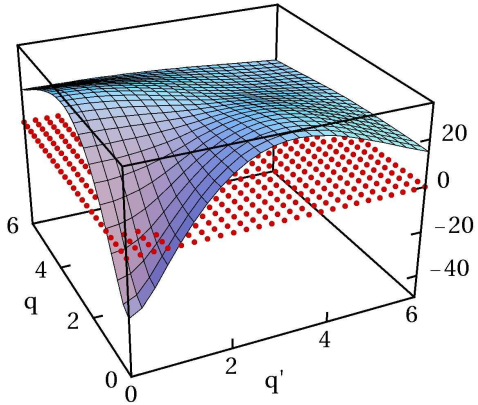
- The correlation functions are determined once for each (S, T) channel by minimizing the energy of the two-body system

- Operators for all observables can (and have to) be correlated consistently

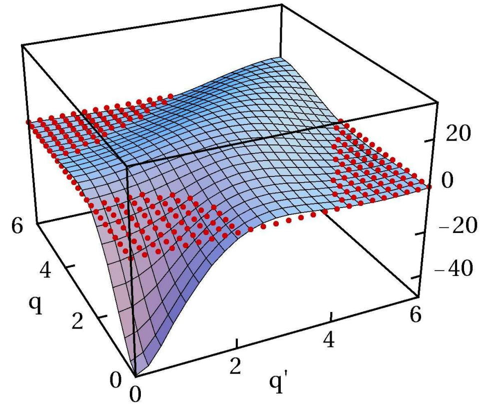
Argonne V18 potential

$$\langle q(LS)J|V|q'(L'S)J\rangle$$

$^1S_0$

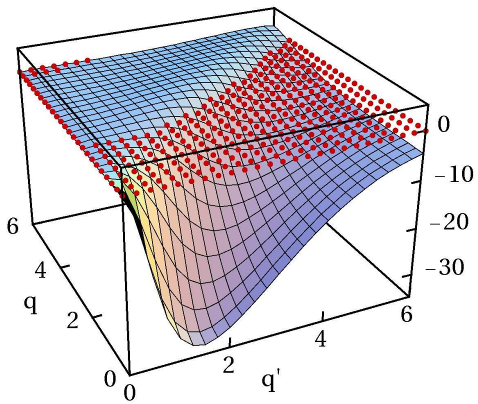


$^1S_0$

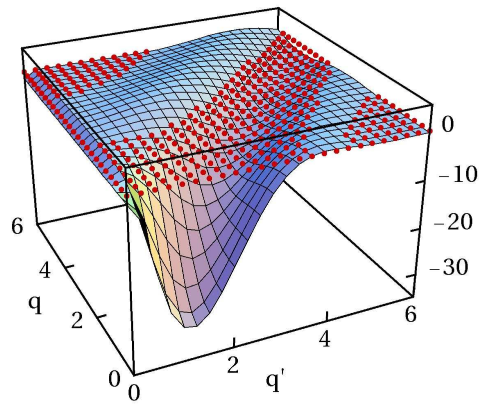


$\leftarrow$ **bare** vs **correlated** $\rightarrow$

$^3S_1 - ^3D_1$



$^3S_1 - ^3D_1$



$[q, q'$ in fm$^{-1}]$

Correlated Hamiltonian and missing pieces

- Cluster expansion: $\hat{H} = C^\dagger H C = \hat{H}^{[1]} + \hat{H}^{[2]} + \hat{H}^{[3]} + \cdots$

- Only short-range correlations are treated by the UCO C

  ➥ Two-body approximation: $\hat{H} \approx \hat{H}^{C2} = \hat{H}^{[1]} + \hat{H}^{[2]}$

- Long-range correlations should be described by the model space

——-

✗ Missing: Three-body forces & correlations

Genuine and due to truncation of cluster expansion - to be quantified

Possibility to introduce additional phenomenological tree-body correction term

Few-body calculations within the No-Core Shell Model

Ground state of ^{4}He: Argonne V18

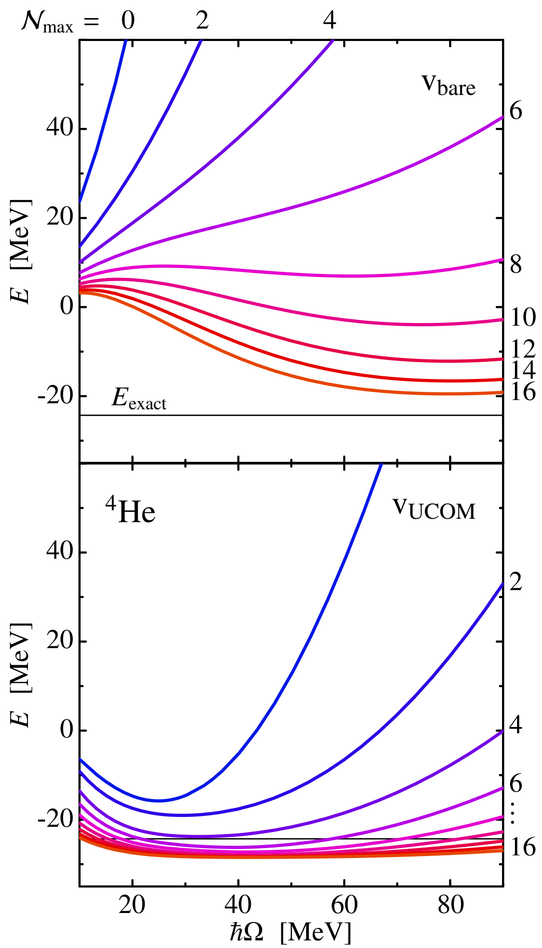
bare interaction

Slow convergence vs $\mathcal{N}_{\max} = (2n + \ell)_{\max}$

correlated interaction `AV18_corintE1009`

Convergence for small spaces

at value lower than exact value E_{exact}



[Numerical code: P. Navrátil *et al.*, PR**C61** (2000) 044001]

UCOM matrix elements & applications

- Harmonic Oscillator Basis: two-body matrix elements in analytical form

  calculated separately and stored; same for all nuclei considered
- UCOM interaction + K.E. + Coulomb: HF with finite-range forces
- Plus long-range correlations
  - Perturbation theory
  - RPA

    Correlation energy

    Excitation strength distributions
  - Extended RPA - built on the RPA ground state ; formulated in the natural-orbital basis and solved iteratively

    New excitation strength distributions

➜ Second RPA

➜ ... HFB, QRPA, CCM, shell model ...

UCOM::Hartree-Fock

- Ground state approximated by a Slater Determinant

$$|\mathrm{HF}\rangle = \mathcal{A}\{|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots |\phi_A\rangle\}$$

- Single-particle states are expanded in a H.O. basis

$$|\phi_i\rangle = \sum_\alpha D_{i\alpha}|\alpha\rangle \qquad ; \qquad |\alpha\rangle = |n, (\ell\tfrac{1}{2})jm, \tfrac{1}{2}m_t\rangle$$

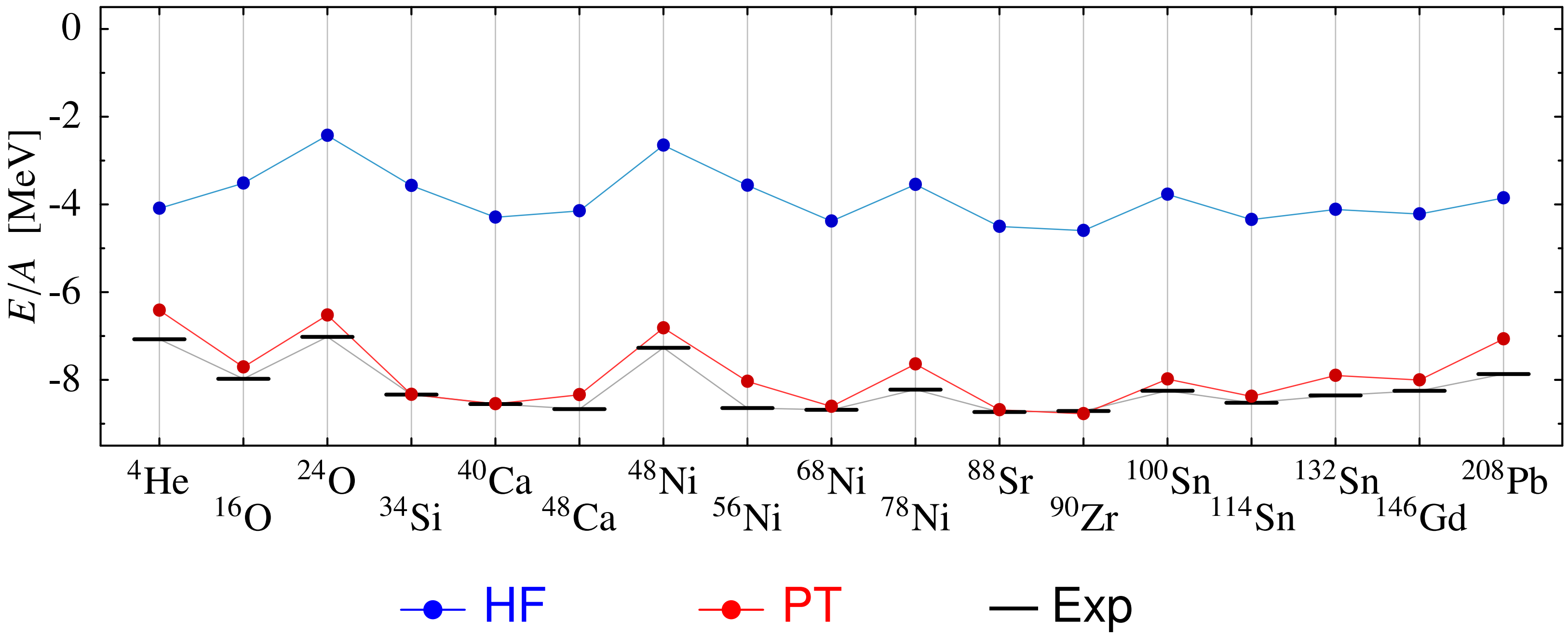
- Expansion coefficients $D_{i\alpha}$ determined by minimizing the energy

$$E_{\mathrm{HF}} = \langle \mathrm{HF}|\hat{H}|\mathrm{HF}\rangle = \begin{cases} \sum_{i=1}^{A} \langle\phi_i|t|\phi_i\rangle + \frac{1}{2}\sum_{i,j=1}^{A}\langle\phi_i\phi_j|V|\phi_i\phi_j\rangle \\ \text{or:} \quad \frac{1}{2}\sum_{i,j=1}^{A}\langle\phi_i\phi_j|T_{\mathrm{rel}} + V|\phi_i\phi_j\rangle \end{cases}$$

UCOM::HF+Perturbation theory

Second-order perturbation theory : $\Delta E^{[2]} = -\frac{1}{4} \sum_{i,j}^{\text{occ}} \sum_{a,b}^{\text{unocc}} \frac{|\langle ij|V_{\text{UCOM}}|ab\rangle|^2}{e_a + e_b - e_i - e_j}$

Binding energies



UCOM::HF+RPA

- Vibration creation operator:

$$Q_\nu^\dagger = \sum_{ph} X_{ph}^\nu O_{ph}^\dagger - \sum_{ph} Y_{ph}^\nu O_{ph} \quad ; \quad Q_\nu |\mathrm{RPA}\rangle = 0 \quad ; \quad Q_\nu^\dagger |\mathrm{RPA}\rangle = |\nu\rangle$$

- Standard RPA - the RPA vacuum is approximated by the HF ground state:

$$|\mathrm{RPA}\rangle \rightarrow |\mathrm{HF}\rangle \quad ; \quad O_{ph} \rightarrow a_p^\dagger a_h$$

- RPA equations in $ph-$space:

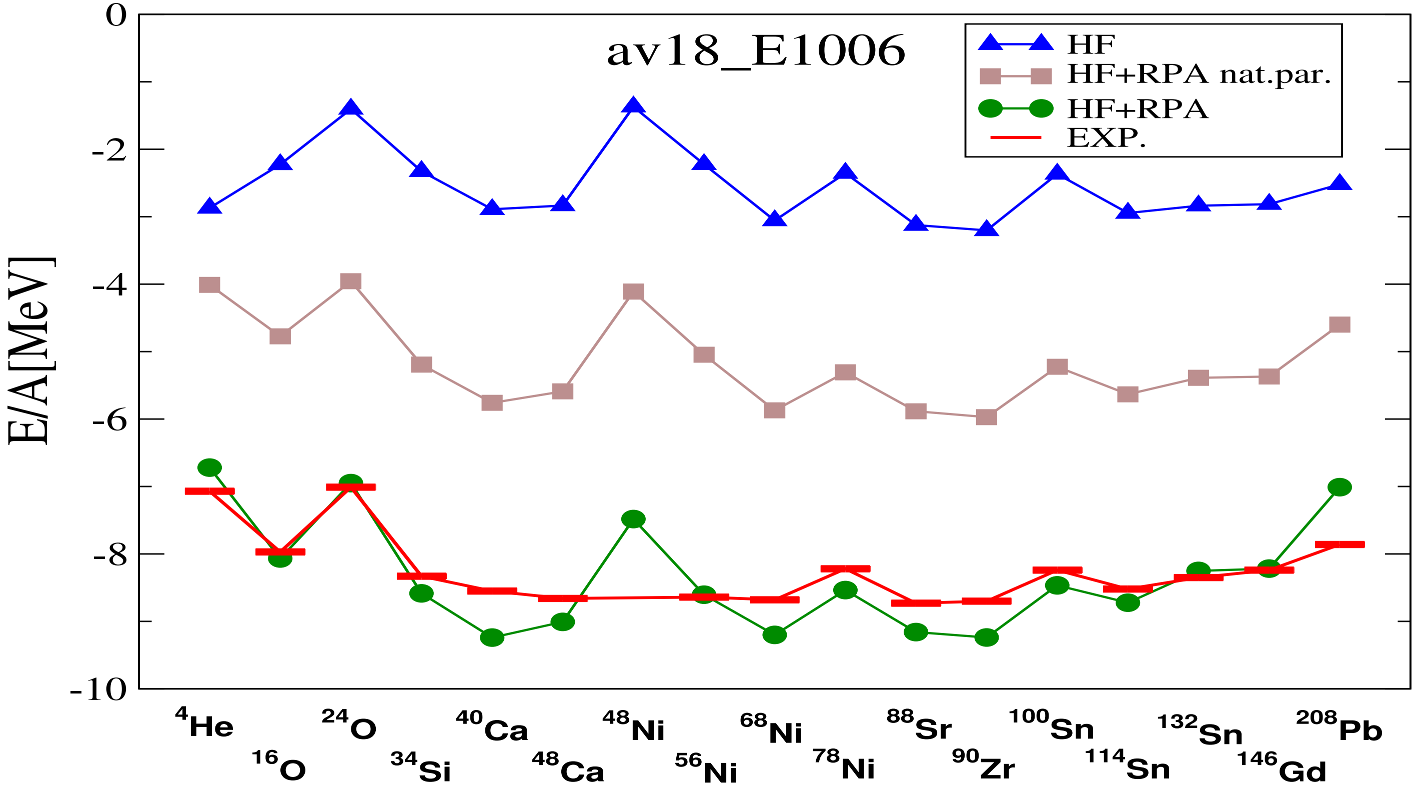
$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \hbar\omega_\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}$$

$$A_{ph,p'h'} = \delta_{pp'}\delta_{hh'}(e_p - e_h) + H_{hp',ph'} \quad ; \quad B_{ph,p'h'} = H_{hh',pp'} \quad ; \quad H = T_{\mathrm{rel}} + V$$

- Self-consistent HF+RPA

UCOM::HF+RPA

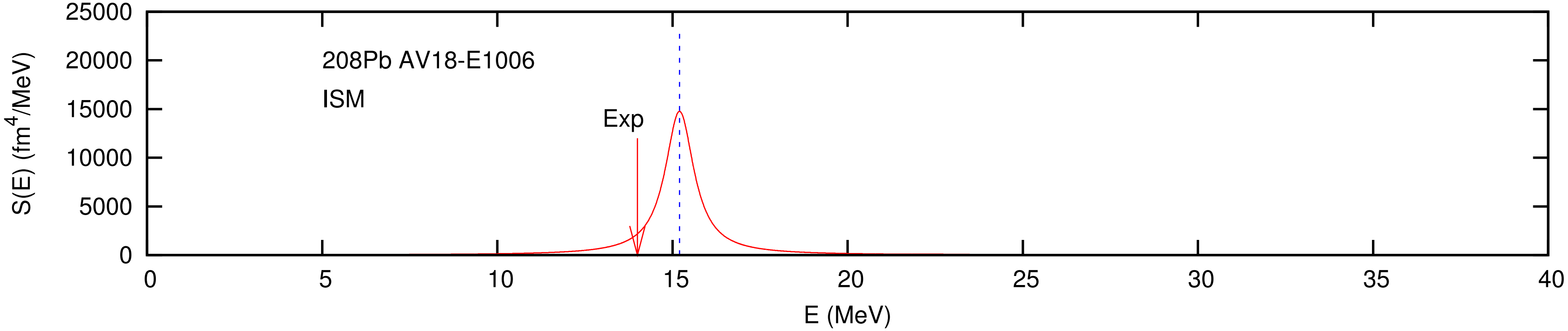
Correlation Energy: $\Delta E_{\mathrm{RPA}} = -\sum_{\nu}(2J+1)\hbar\omega_{\nu}\sum_{ph}|Y_{ph}^{\nu}|^2$



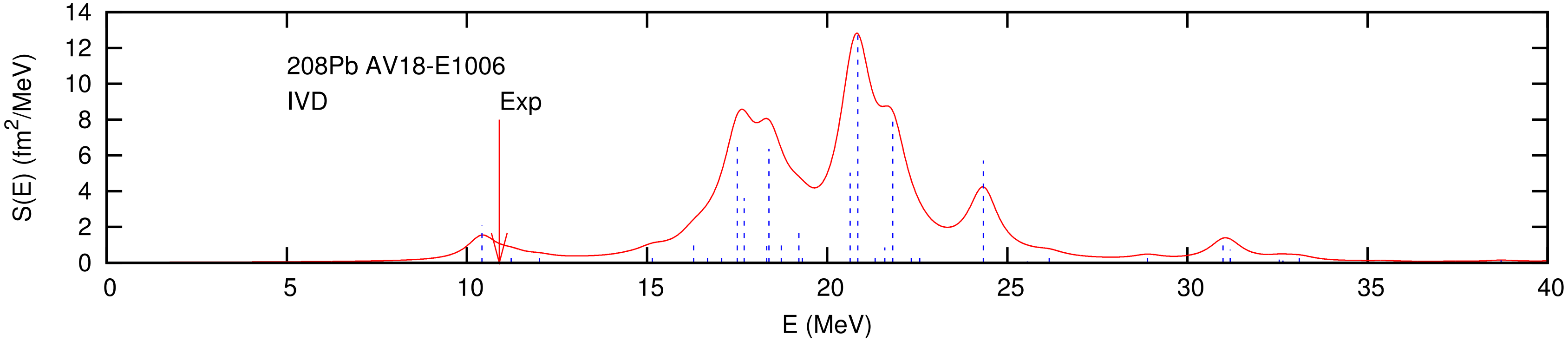
UCOM::HF+RPA

208Pb – Prelim:AV18-E1006

ISM:

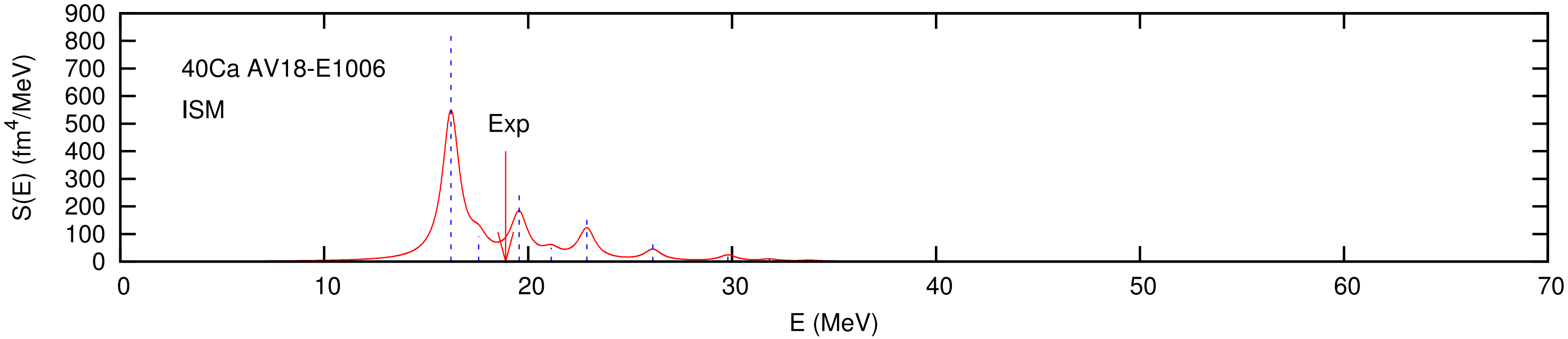


IVD:



40Ca – Prelim:AV18-E1006

ISM:



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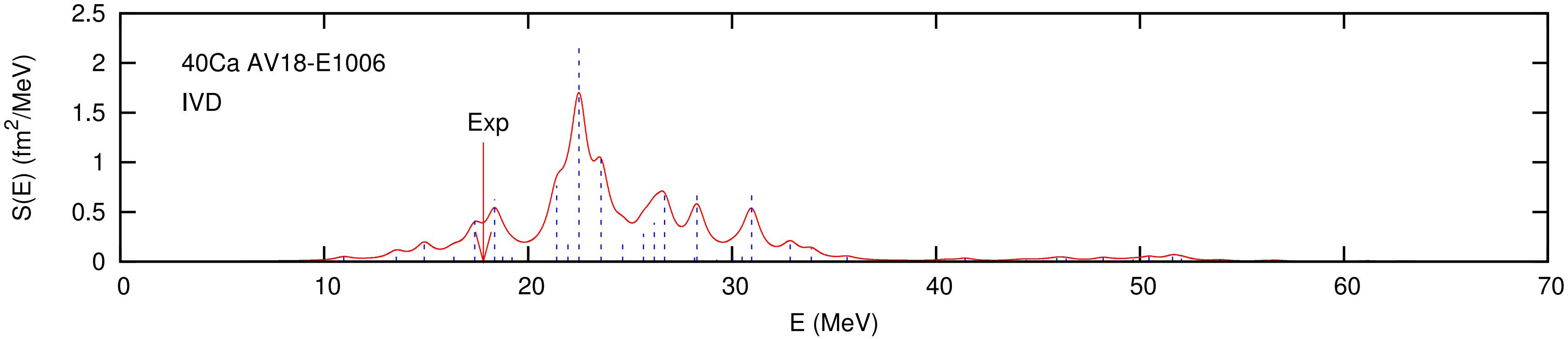


UCOM::ExtendedRPA

- Excitations are built on the RPA vacuum. In general,

$$O_{ph} = \sum_{p'h'} N_{ph,p'h'} a^{\dagger}_{p'} a_{h'}$$

- ERPA formulated in the natural-orbital basis

$$O_{ph} \rightarrow D_{ph}^{-1/2} a^{\dagger}_{p} a_{h} \quad ; \quad D_{ph} \equiv n_h - n_p$$

- ERPA equations: solved iteratively

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix} = \hbar\omega_{\nu} \begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix}$$

$$A_{ph,p'h'} = \delta_{hh'} e_{pp'} - \delta_{pp'} e_{hh'} + D_{ph}^{1/2} D_{p'h'}^{1/2} H_{hp',ph'} \quad ; \quad B_{ph,p'h'} = D_{ph}^{1/2} D_{p'h'}^{1/2} H_{hh',pp'}$$

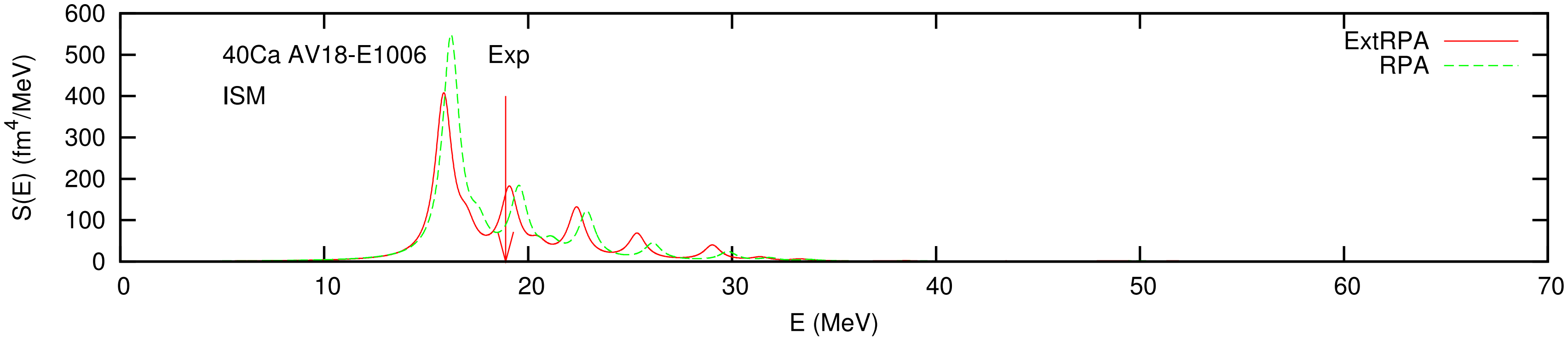
$$e_{ij} = t_{ij} + \sum_{k} n_k H_{ik,jk}$$

[Catara et al.: PRB58(98)16070; Voronov et. al.: Phys.Part.Nucl.31(00)904]

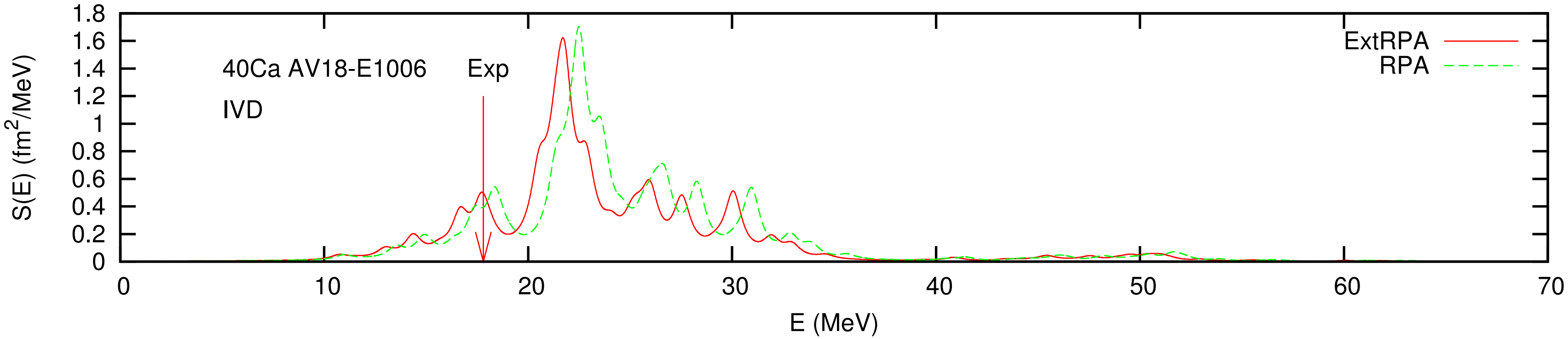
UCOM::Extended RPA

40Ca – Prelim:AV18-E1006

ISM:



IVD:



Summary - Perspectives

- The UCOM provides us with effective interactions based on realistic NN potentials
  - in tractable analytical form
  - same for all nuclei
  - suitable for simple Hilbert spaces
- Hartree-Fock + long-range correlations: PT, RPA, ERPA
  - Properties of ground states and excitations
  - Promising results
  - Optimization of tensor-correlation range

✎ SRPA, HFB+QRPA, ... to be continued